Karl K. Irikura

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Education

Ph.D. in Chemistry — December 1990
California Institute of Technology, Pasadena, California
Thesis: *Gas-Phase Chemistry of Organotransition Metal Ions*
Advisor: Prof. J. L. Beauchamp

A.B. in Chemistry (*summa cum laude)* — June 1984
Harvard College, Cambridge, Massachusetts

Awards

Sigma Xi Young Scientist Award (NIST chapter) (1998)
National Research Council Research Associateship (6/91-6/93)
National Science Foundation Predoctoral Fellowship (9/84-9/87)

Experience

Government Research

Conducted *ab initio* calculations to identify and solve problems in thermochemistry, chemical kinetics, and molecular spectroscopy. Developed computational techniques for reaction energetics and spectroscopy. (National Institute of Standards and Technology, 6/93-present)

Postdoctoral Research

Conducted exploratory studies and characterization of free radicals and other reactive intermediates using resonance-enhanced multiphoton ionization spectroscopy. Employed *ab initio* calculations to clarify and extend spectroscopic results. (J. W. Hudgens, National Institute of Standards and Technology, 7/91-6/93)

Used advanced *ab initio* quantum chemical techniques to study the structure and energetics of reactive organometallic and bio-organic species. (W. A. Goddard III, California Institute of Technology, 1/91-6/91)

Graduate Research

Studied numerous metal-containing ions using both experimental and theoretical techniques. Employed Fourier-transform mass spectrometry to study thermochemistry and reactivity of organometallic, inorganic, and bio-inorganic ions in the gas phase. Addressed questions in interstellar chemistry and physical organic chemistry using quantum and classical theoretical methods. (J. L. Beauchamp, California Institute of Technology, 9/84-12/90)

Undergraduate Research

Conducted molecular dynamics calculations on B- and Z-DNA oligomers. (M. Karplus, Harvard, 2/83-6/84)

Synthesized substituted acridines. (S. A. Benner, Harvard, 2/82-6/82)

Industrial Research

Investigated kinetics of olefin hydroformylation catalyzed by soluble rhodium complexes. (A. A. Oswald, Exxon Research and Engineering Co., Summer 1983)

Studied alkane dehydrocyclization and aromatization over zeolite-supported platinum catalysts. (S. J. Tauster, Exxon Research and Engineering Co., Summer 1982)

Teaching

Delivered lectures and laboratory course on *ab initio* thermochemistry (NATO ASI, Castelo Branco, Portugal, 7/98)

Teaching assistant for biophysical chemistry (two years) and for freshman chemistry (three years). Duties included grading, classroom teaching, demonstrations, and composition of problem sets and examinations. (California Institute of Technology, 9/84-6/89)

Grading for general chemistry and laboratory preparation for organic chemistry course with 350 students. (Harvard, 9/83-6/84)

Technical Skills

Ab Initio Software: GAUSSIAN (J. A. Pople *et al.*), GAMESS-USA (M. S. Gordon *et al.*), MOLCAS (B. O. Roos *et al.*), ACES II (R. J. Bartlett *et al.*), MOLFDIR (W. C. Nieuwpoort *et al.*), MOLECULE-SWEDEN (J. Almlöf *et al.*), MQM (W. A. Goddard III *et al.*), COLUMBUS (R. Shepard *et al.*)
Computers: Experience with Perl, awk, C, Fortran, Basic, Pascal, Java, assembler
Resonance-Enhanced Multiphoton Ionization Spectroscopy
Fourier-Transform Ion Cyclotron Resonance Spectrometry (FTMS)
Lasers: Excimer, dye, Nd:YAG, CO_2
Vacuum Technology: Ultrahigh vacuum methods and equipment, pulsed valves, TOF-MS.
Foreign Languages: Written and spoken French (intermediate) and German (weaker)

Professional Service

Organizing committee, NATO Advanced Study Institute, "Energetics of Stable Molecules and Reactive Intermediates," Castelo Branco, Portugal, July 14 - 24, 1998.
Organizer, symposium on "Computational Thermochemistry," 212th ACS National Meeting, Orlando, Florida, August 25-29, 1996.

Publications

Technical Presentations